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ABSTRACT

A constrained component analysis method, which bears a formal resemblance to the confirmatory factor analysis methods developed by K. G. Joreskog (1969) and others, is presented. In confirmatory factor analysis, the constraints allow the testing of formally structural hypotheses within a model that is falsifiable, even in its "just defined" form. In component analysis, the goal is to determine whether a component solution that is restricted in various ways can still account for an adequate share of the variance in the observed data. The consistency and efficiency of the estimates under the constrained analysis are considered; however, no statistical tests of fit of the component are discussed. In this sense, the method is closer to the work in constrained canonical correlation by W. S. DeSarbo and others (1982). Interesting applications of constrained component analysis exist in data that are longitudinal or cross-sectional in nature. In these cases, the natural constraints may involve the property of being stationary or the invariance of the compositing weight, component pattern, or component structure matrices. In data measured at a single occasion in a single population, constraints might be used to impose simple structure or achieve a sensible variable clustering. Boundary constraints might be used to achieve a positive manifold. (TJH)

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Component Analysis under Linear Equality and Inequality Constraints

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A paper by Meredith & Millsap (1985) presented a view of component analysis in which the regression of observed on component variables plays the central role. In this regression, the "adequacy" of a component representation is measured by the amount of error in the least-squares approximation of observed by component variables. Let X be an nx1 vector of observed random variables, with $\epsilon(X)=0$ and $\epsilon(XX')=\Sigma$. To simplify discussion, we assume rank(Σ)=n. Let $Z=W'X$ be an mx1 vector of component random variables, with W an nxm compositing weight matrix to be applied to the observed variables. The paper by Meredith & Millsap (1985) demonstrated that using a weighted squared error loss function, the optimal component solution is given by the matrix W which maximizes the function

$$F(W;\Sigma,G) = tr\{W'\Sigma G\Sigma W(W'\Sigma W)^{-1}\}. \qquad (1)$$

The matrix G is an nxn nonsingular matrix that can be used to differentially weight the elements of X in deriving the components. Weighted component analysis is discussed in Mulaik (1972). Meredith & Millsap (1985) give an extensive discussion of possibilities for weighting.

Note that the value of (1) cannot exceed $tr\{G\Sigma\}$. A natural measure for the adequacy of a component solution is the ratio of (1) to $tr\{G\Sigma\}$. This ratio will be unity if m=n, and will approach unity for m<n as the component solution accounts for a greater share of the observed variance.

Component Analysis under Linear Constraints

Before introducing linear constraints in the component analysis, it will be useful to rewrite (1) in a slightly more general form

$$H(U;A,B) = tr\{U'AU(U'BU)^{-1}\} \qquad (2)$$

with A and B both qxq matrices of rank q, and U a qxs matrix. Clearly, (1) is the special case of (2) in which q=n, s=m, $A=\Sigma G\Sigma$, and $B=\Sigma$.

A solution for U which maximizes H(U; A, B) is found as follows. Factor $B=LL'$ and let $A^*=L^{-1}AL'^{-1}$, $U^*=L'U$. Then

$$H(U;A,B) = H(U^*;A^*,I) = tr\{U^{*\prime}A^*U^*(U^{*\prime}U^*)^{-1}\} \qquad (3)$$

Let the spectral representation of $A^*=Q\Lambda Q'$. A theorem by Bellman (1960) gives the matrix U^* which maximizes (3) as $U^*=Q_mT$, where Q_m is an nxm matrix whose columns are the m eigenvectors corresponding to the m largest eigenvalues of A^*, and T is any mxm nonsingular matrix. The solution identifies a class of matrices U^*, and we must choose a matrix T to identify a member of this class.

In terms of the function F(W; Σ, G), let $\Sigma=LL'$, $W^*=L'W$, and $A^*=L^{-1}\Sigma G\Sigma L'^{-1}$. If the spectral representation of $A^*=Q\Lambda Q'$, the solution for $W^*=Q_mT$ and $W=L'^{-1}Q_mT$. We typically choose T to be an identity matrix or a diagonal matrix of the reciprocal square roots of the first m eigenvalues.

To introduce the constrained solution to (2), consider concatenating the columns of $U=[u_1, u_2, \ldots, u_s]$ to form a column vector V such that $V'=[u_1', u_2', \ldots, u_s']$. We want to find a matrix U which maximizes (2) under the constraints

$$C'V \geq M \qquad (4)$$

with C a qsxr nonsingular matrix and M an rx1 vector. Some or all of the r constraints in (4) may be taken as equalities, but the number of equality constraints may not exceed qs. The constraints in (4) can be used to fix elements of U to selected values, to equate elements of U,

to set lower or upper bounds on the elements of U, or to fix linear composites of the elements of U to selected values. We can employ some of the constraints in (4) for purposes of identifying U. For this purpose, s^2 equality constraints are sufficient.

Structure and Pattern Matrices

We began with a description of component analysis that focused on the compositing matrix W. Given a solution for W, we can define the component pattern matrix $P=\Sigma W(W'\Sigma W)^{-1}$ and the component structure matrix $R=\Sigma W$. Note that we can write the function H in terms of W, P, or R

$$H(W;\Sigma G\Sigma,\Sigma) = tr\{W'\Sigma G\Sigma W(W'\Sigma W)^{-1}\} \quad (5)$$

$$H(P;G,\Sigma^{-1}) = tr\{P'GP(P'\Sigma^{-1}P)^{-1}\} \quad (6)$$

$$H(R;G,\Sigma^{-1}) = tr\{R'GR(R'\Sigma^{-1}R)^{-1}\} \quad (7)$$

Clearly, constriants of the form in (4) can be applied to either (6) or (7) as well as (5). In other words, we can derive components whose pattern or structure matrices conform to specified constraints.

Extrema of the Function

The unconstrained function H(U;A,B) is continuous and has $\binom{n}{m}$ stationary points, with both a unique global maximum and a unique global minimum, assuming distinct eigenvalues for the matrix A^*. In practice therefore, H(U;A,B) is bounded. If we impose m^2 equality constraints in (4) to identify U, the matrices U which satisfy these constraints constitute a closed, bounded convex set. Hence there must exist both a global maximum and a global minimum for H over this set. The addition of further equality or inequality constraints will not alter the existence of a global maximum, but the maximum may no longer

be unique. In general, if additional constraints are imposed, the maximum value for H achieved under these constraints will be less than that under the "just identified" solution.

The Adequacy of the Constrained Solution

We can evaluate the adequacy of the constrained component solution in at least two ways. An "absolute" measure of adequacy can be calculated by replacing the solution for W, P, or R in (5), (6), or (7) respectively. Then either (5), (6), or (7) can be divided by $tr\{G\Sigma\}$. This ratio measures the variance "accounted for" by the constrained solution against the total variance observed. Alternatively, we could calulate a "relative" measure of adequacy by dividing the value of H under the constrained solution by the value of H under a "just identified" solution. Here we are measuring the variance accounted for by the constrained solution against the variance accounted for by the "just identified" solution. If this ratio is near unity, we can be confident in using the constrained solution in place of the principal component solution.

Final Remarks

The constrained component analysis method presented here bears a formal resemblance to the confirmatory factor analysis methods developed by Joreskog (1969) and others. In confirmatory factor analysis, the constraints allow us to formally test structural hypotheses within a model that is falsifiable, even in its "just identified" form. In component analysis, the goal is to determine whether a component solution that is restricted in various ways can still account for an adequate share of the variance in the observed data. We may also be

concerned with the consistency and efficiency of the estimates under the constrained analysis. But no statistical tests of fit of the component "model" are contemplated. In this sense, the method presented here is closer to the work in constrained canonical correlation by DeSarbo, Hausman, Lin, & Thompson (1982) than to confirmatory factor analysis.

Interesting applications of constrained component analysis exist in data that is longitudinal or cross-sectional in nature. In these cases, the natural constraints may involve stationarity or invariance of the compositing weight, component pattern, or component structure matrices. In data measured at a single occasion in a single population, constraints might be used to impose simple structure or achieve a sensible variable clustering. Boundary constraints might be used to achieve a positive manifold.

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